A New Functional Form and Fitting Techniques for Equations of State with Application to Pentafluoroethane (HFC-125)

E.W. Lemmon [C, S]
Physical and Chemical Properties Division, National Institute of Standards and Technology, Boulder, CO, U.S.A.

R.T Jacobsen
Idaho National Engineering and Environmental Laboratory, Idaho Falls, ID, U.S.A.

A widely used form of an equation of state explicit in Helmholtz energy has been modified with new terms to eliminate certain undesirable characteristics in the two phase region. All modern multiparameter equations of state exhibit behavior in the two phase region which is inconsistent with physical fluid behavior. Calculated values of pressure may exceed in some cases $1x10^{20}$ MPa, and large negative pressures are common. The new functional form overcomes this dilemma and results in better equations of state for pure fluids, particularly for mixture modeling. With the addition of certain nonlinear fitting constraints, the new equation now achieves proper phase stability, i.e., only one solution exists for phase equilibrium for each phase equilibrium state. This condition has never been satisfied in previous multiparameter equations of state. New fitting techniques have been implemented to ensure proper extrapolation of the equation at low temperatures, in the vapor phase at low densities, and at very high temperatures and pressures.

A formulation is presented for the thermodynamic properties of refrigerant R125 (pentafluoroethane, CHF2-CF3) using the new terms and fitting techniques. The equation of state is valid for temperatures from the triple point temperature (172.52 K) to 500 K and for pressures up to 60 MPa. The formulation can be used for the calculation of all the thermodynamic properties, including density, heat capacity, speed of sound, energy and saturation properties. Comparisons to available experimental data are given that establish the accuracy of calculated properties using this equation of state. The estimated uncertainties of properties calculated using the new equation are 0.1% in density, 0.5% in heat capacities, 0.01% in the speed of sound for the vapor at pressures less than 1 MPa, 0.5% in the speed of sound elsewhere, and 0.1% in vapor pressure. Deviations in the critical region are higher for all properties except vapor pressure.